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MOLECULAR DYNAMICS NUCLEATION AND OCCURRENCE PROCESSES OF PHASE TRANSITIONS IN DISORDERED SYSTEMS

Specialization 01.04.02 – Theoretical physics

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GENERAL CHARACTERISTICS

Actuality of the work. The problem of numerical evaluation the characteristics of the phase transitions in condensed systems is one of the most actuality. According to the classical nucleation theory the phase transition begins when the so-called critical clusters of new phase are emerging as a result of random fluctuations in system. Identify these clusters is extremely difficult by experimental methods of structural analysis. The reason for this is the small size the new phase clusters. Also, there are no detailed studies of nucleation processes in amorphous systems at deep supercooling. Here, the detect of universal laws in the temperature behavior of the main kinetic nucleation parameters (the steady-state nucleation rate, induction time, cluster growth rate) is necessary. The define the numerical values of these parameters is impossible by experimental methods. Therefore a method of molecular dynamics simulation allows accurately calculate any features of phase transitions in condensed systems.[1]

The molecular dynamics simulation of various structural transformations in condensed systems by coarse-grained interaction potentials is most actual. In particular, there is a need to reconstruction of effective potentials for describing the physical properties and structural characteristics of the systems as water, salt solutions, multi-component materials, metal alloys etc.[2] For example, recently the description of kinetic and thermodynamic characteristics of the saturated vapor at condensation by coarse-grained models was absent. As a rule, in most works, which are devoted to the study of the properties of water by means of molecular dynamics simulations the atomistic potentials as a TIP4P, SPC/E are used.

Another actual problem is related to the study of crystallization mechanisms in disordered systems under the external influences. The

[1] D. Kashchiev *Nucleation: Basic Theory with Applications* (Butterworth-Heinemann, Frenkel Oxford, 2000).

[2] D. Frenkel, and B. Smit *Understanding Molecular Simulation* (San Diego: Academic Press, 2001).

detailed explanation and analysis of experimental data for crystallization processes at shear deformation is required, e.g. in case of polymers and colloidal suspensions. Understanding of the influence of shear deformation on the crystal nucleation process in amorphous materials is also absent. It should be noted that the classical nucleation theory does not explain all of the features observed in the experiment. It is clear that the understanding of these processes will contribute to the development of management techniques the occurrence of phase transitions.

The goal of the work is study the nucleation and occurrence processes of phase transition in disordered systems by methods of equilibrium and nonequilibrium molecular dynamics simulations.

The scientific novelty of the work consists in the following:

1. An original method of structural analysis of the molecular dynamics simulation results was proposed. This method is allowed to evaluate the three-particle correlations in condensed systems.

2. An original approach, which based on the method of thermodynamic integration was proposed. This approach is allowed to estimate the surface tension of the critical nuclei.

3. The original temperature scale was introduced for the temperature range of $0 < T \leq T_m$ (the quantity T_m is the melting temperature). This temperature scale can be used as an alternative to, for example, supercooling and/or reduced temperature (e.g. so-called Angell plot).[3]

4. The numerical calculations of the structural and dynamic characteristics of the model glasses were performed by method of molecular dynamics simulation at deep supercooling.

5. The characteristics of crystallization of the model glasses were calculated by method of nonequilibrium molecular dynamics simulation at external homogeneous shear.

[3]C.A. Angell // Science. - 1995. - Vol. 267, P. 1924.

6. The temperature dependencies of the kinetic and thermodynamic characteristics of condensation of the supersaturated vapor were calculated on the basis of coarse-grained water model.

Scientific and practical value. The results of a large-scale equilibrium and nonequilibrium molecular dynamics simulation make a significant contribution to the understanding the mechanisms of phase transitions in disordered systems. The original approaches will be very useful in the development of methods for the analysis of structural and mechanical properties of solids and liquids. The results of this work are contribute to understanding of the mechanisms of nucleation processes in disordered systems at different levels of metastability. Also, these results can be very useful in the design and development of practical methods of influence on the course of phase transitions.

The main provisions:

1. A method of structural analysis allows to obtain information about the evolution of the three-particle correlations in multiparticle systems on the basis of molecular dynamics simulation.

2. The mechanism of homogeneous crystal nucleation is observed in the case of equilibrium and nonequilibrium phase transitions in the one-component and two-component glass systems at deep supercooling.

3. The procedure of thermodynamic integration allows to calculate the thermodynamic properties of phase transitions: the interfacial free energy, surface tension, nucleation barrier, in the framework of molecular dynamics simulation.

4. In the case of homogeneous nucleation at temperatures from 0°C to 100°C the growth of water droplets is accelerated. The droplet growth laws are independent on the system temperature.

Presentation of the work. The main results and conclusions of this work were presented at the International Scientific School of

modern neutron diffraction (Dubna, JINR, 2012); International scientific internet-conference "Mathematical and computer modeling in biology and chemistry. Prospects for future developments" (Kazan, KFU, 2012); The conference "Irreversible processes in nature and technology" (Moscow, MSU, 2013, 2015); The International Internet-conference "On the intersection of science. Physico-chemical series" (Kazan, KFU, 2013, 2015); The conference "Materials and Technologies of XXI century" (Kazan, KFU, 2014); The XVIIIth Research Workshop "Nucleation Theory and Applications" (Dubna, JINR, 2014); International Science Forum "Lomonosov -2015" (Moscow, MSU, 2015); XIV International School-conference "The problems of solid state physics and high pressure" (Sochi, IHPP RAS, FIAN, 2015); I International School-Conference for Young Scientists "Biomedicine, materials and technologies of the XXI century" (Kazan, KFU, 2015), in the conferences of department of the computational physics in Institute of physics KFU (2011-2015).

Publications. The results of the research were published in 19 publications, 6 of them in scientific journals, included in the citation database Scopus, Web of Science, and eLibrary, 3 articles in collections of scientific papers, 10 abstracts on international and national scientific conferences. The 6 certificates of state registration and accounting software systems for computers were obtained.

Structure of the manuscript. The PhD thesis consists of five chapters, conclusion and list of references. The work is described in the 179 pages that include 46 graphics, 15 tables, and 180 items of cited literature.

CONTENT

In the introduction the relevance of the investigated problem is argued, the scientific and practical significance of the work are justified, the purpose of the study and the provisions for the defense are stated, as well as set out the structure and content of this work.

In the first chapter the main algorithms of molecular dynamics simulation within pair and three-particle potentials of interatomic or intermolecular interaction are presented. It was shown that the molecular dynamics calculations with the effective potential allow to reproduce the structural characteristics of condensed systems. By method of molecular dynamics simulation was reconstructed the effective coarse-grained interaction potential for water. It is shown that the Stillinger-Weber potential can be adapted to reproduce the structural properties of water in the temperature from 0°C to 100°C. In this model the water molecule is considered as a separate particle, while the interaction between oxygen and hydrogen atoms is considered effective manner. The results are showed that in the effective potential, which was proposed earlier by E.B. Moore and V. Molinero the optimal parameter values are used.[4]

In the second chapter the known and original methods of describe the phase transitions in condensed systems are considered. The methods of cluster and structural analysis are used through statistical analysis of the results of molecular dynamics simulation. It was shown that the original methods are adequately interpreted the results of molecular dynamics simulation and experimental data.

To assess the nucleation parameters such as size critical nucleus n_c, the stationary nucleation rate J_{st}, nucleation time scale, nucleation barrier, was proposed an original method of inverted averaging. This method allows to analyze the average time of the appearance of both the first and subsequent nucleation events (appearance of critical nuclei) from the results of molecular dynamics simulation. It is shown that the numerical values of the steady-state nucleation rate J_{st} can be evaluate from the analysis of the evolution the quantity of the supercritical nuclei $n > n_c$.

A new approach for calculation the surface tension σ_s of critical size nuclei is presented. The need in this approach is caused due to the lack of adequate methods to assess the interfacial characteristics from

[4]E.B. Moore and V. Molinero // Nature. - 2011. - Vol. 479, P. 506-508.

the results of molecular dynamics simulation. The advantage of this approach is that the value of σ_s can be calculated for the critical nuclei, the surface of which is characterized by significant curvature. Here, the surface tension of the critical nucleus at different numerical experiments M is estimated as

$$\sigma_s = -\int_0^1 \left\langle \frac{\partial \omega(\lambda)}{\partial \lambda} \right\rangle_M d\lambda. \tag{1}$$

The excess energy ω per unit surface is given by equation

$$\omega = \frac{1}{2} u_{II}(r)[z_v - z_s]n_s. \tag{2}$$

Here, $u_{II}(r)$ is the potential energy of interaction between the two neighboring particles (atoms or molecules or ions) a new phase at a distance r from each other [5]; $\lambda = \sqrt[3]{n/n_c}$ is the defined as the ratio of the size n to the critical size n_c. The quantity n_s is the surface particles per unit the surface area of the nucleus; z_v and z_s are the first coordination numbers for the volume and surface particles, respectively.

An original method for analyzing the evolution of the three-particle correlations was proposed for study the three-particle interactions in many-body systems . The consideration of only the pair correlation does not allow to fully explain and describe effects such as the formation of orientational ordering in quasicrystals, occurrence of dynamic inhomogeneities in liquids etc. Traditionally the two parameters (for example, the distance between the particles, angles) are used for a description of physical process. In proposed method the original three-particle correlations are described by a single parameter - triangle with area S, which formed by three arbitrary particles.

For the study of three-body relaxation processes used autocorrelation function as

$$F_T(k,t) = \frac{1}{N_T} \sum_{j=1}^{N_T} \exp\left[-i\vec{k}\vec{s}_j(t)\right], \tag{3}$$

[5] J.I. Frenkel *Kinetic Theory of Liquids* (L. Science, 1975)

$$\vec{s}_j(t) = \frac{\mu_j S_j(t) \vec{N}_j}{\sigma}. \tag{4}$$

Here, $\vec{k}$ is the wave vector, σ is the particle diameter, $\vec{N}_j = n_1(j)\vec{e_x} + n_2(j)\vec{e_y} + n_3(j)\vec{e_z}$ is the normal to the plane of the jth triangle, N_t is the number of triangles, $S_j(t)$ is the area of jth triangle at time t, $\mu_j = \pm[n_1^2(j) + n_2^2(j) + n_3^2(j)]^{-1/2}$ is the normalization constant, which is determined by the sign n_4 in the equation $n_1(j)x + n_2(j)y + n_3(j)z + n_4(j) = 0$. It was found that the solution of equation

$$\ddot{F}(k,t) + \Omega_1^2(k)F(k,t) + \varphi(k)\dot{F}(k,t)\delta(t) + \Omega_1^2(k)\int_0^t \left[\upsilon_1 F(k,t-\tau) + \upsilon_2 F(k,t-\tau)^p\right]\dot{F}(k,\tau)d\tau = 0 \tag{5}$$

in the framework of the mode-coupling theory, which allows to reproduce the behavior of three-particle autocorrelation function (3) for liquid and amorphous aluminum in a wide temperature range, as well as the model of a quasicrystal. In equation (5) the value of Ω_1 describes the frequency at which the change area of the triangle, $\varphi(k)$ is the frequency parameter, $\delta(t)$ is the Dirac delta function. The values of $\upsilon_1 \geq 0$ and $\upsilon_2 \geq 0$ are contributions ($\upsilon_1 + \upsilon_2 \neq 0$), where $p > 1$.

By analogy with the radial distribution function for the three-particle structural analysis is applied the equation

$$g(S, r_s) = \frac{\pi r_s^3}{3SN_T}\left\langle \sum_{i=1}^{N_T} \frac{\Delta n_i(S)}{\Delta r_s} \right\rangle. \tag{6}$$

This equation is determine a probability of occurrence of a triangle with area S in the sphere of radius r_s. The value of $\Delta n(S)$ determines distribution over the S. In the figure 1 shows the function $g(S, r_s)$ (under $r_s = 3\,\sigma$ and $\sigma = 0.28\,\text{nm}$) is calculated through the molecular dynamic simulation of amorphous system with 864 aluminum atoms at temperatures of $T = 100\,\text{K}$ and at pressure of $P = 1\,\text{atm}$. In the figure 1 by circles shows a schematic arrangement of the atoms, which contribute to the respective maximum of the function $g(S, r_s)$. We demonstrate

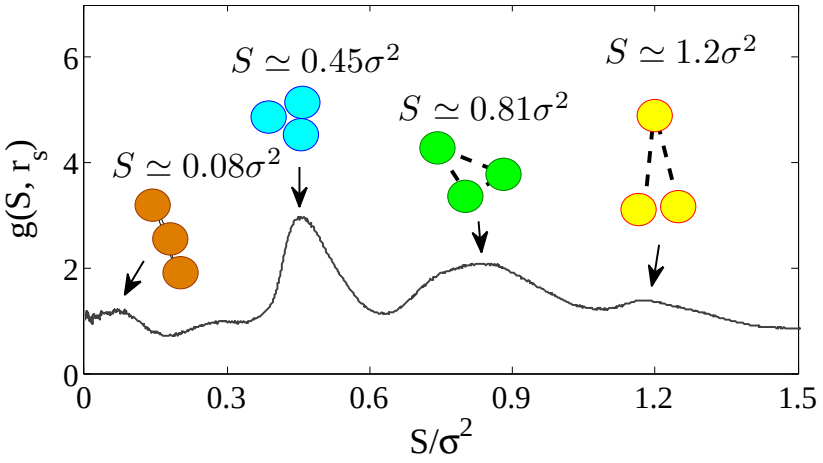

Figure 1: The function $g(S, r_s)$ for amorphous aluminum at $T = 100\,\mathrm{K}$ and at pressure $P = 1\,\mathrm{atm}$. With circles are marked triangles, which characterize the maximums of the function $g(S, r_s)$.

the applicability of the function $g(S, r_s)$ to the structural analysis model liquid, amorphous system, and the model of quasicrystal.

In the third chapter presents the results of molecular dynamics simulation of crystallization process in two different glass systems: one-component Dzugutov system (Dz)[6] and two-component Lennard-Jones system (bLJ)[7]. The temperature regions, which lower than the glass transition point, are considered for both systems. Interest in the study of the crystallization process in these systems is caused by the lack of detailed studies of the nucleation processes at deep supercooling.

The formation of a new phase in the Dz and bLJ-systems is started with the appearance of localized crystalline domains – the nuclei. The average time of the first appearance of larger crystal nucleus was estimate by method of inverted averaging. In addition, the value of steady-state

[6] J. Roth Phys. Rev. B. - 2005. - Vol. 72, P. 014125.
[7] G. Wahnstrom Phys. Rev. A. - 1991. - Vol. 44, P. 3752.

nucleation rate was estimated for the considered temperature range. These results are consistent with the concepts of classical nucleation theory and the experimental data obtained for silicate glasses near the glass transition temperature. It is shown that the critical nuclei are characterized by small size. The calculation of the nonsphericity parameter S_o with value $S_o \simeq 10^{-3}$, which, as it turned out, almost independent of the temperature of the system. Such a value S_o corresponds to spherical shape.

An original method for scaling the absolute temperature scale was proposed for comparison and analysis of simulation results and experimental data. The need for the development of this method due to the fact that in supercooled liquids and glasses the nucleation processes can occur in a temperature range that contains three reference points: zero temperature $T = 0\,K$, the glass transition temperature T_g, and the melting point T_m. In this case the values T_g and T_m may be differ for different systems.

A new temperature scale $\widetilde{T}$ is given by equation

$$\widetilde{T} = \left[\frac{0.5 - \dfrac{T_g^2}{T_m^2}}{1 - \dfrac{T_g}{T_m}} \right] \left(\frac{T}{T_g} \right) + \left[\frac{\dfrac{T_g}{T_m} - 0.5}{\dfrac{T_m}{T_g} - 1} \right] \left(\frac{T}{T_g} \right)^2, \tag{7}$$

which is the equation of the curve passing through the three temperature points: $T = 0\,K$, T_g, and T_m. Expression (7) satisfies the following conditions:

$$\widetilde{T} = 0 \quad \Leftrightarrow \quad T = 0\ K, \tag{8}$$

$$\widetilde{T}_g = 0.5 \quad \Leftrightarrow \quad T = T_g, \tag{9}$$

$$\widetilde{T}_m = 1 \quad \Leftrightarrow \quad T = T_m. \tag{10}$$

In the case when for a system temperatures T_g and T_m are known temperature $\widetilde{T}$ allows to perform a valid comparison of simulation and experimental data for the temperature region $0 < T \leq T_m$, where the temperature points are same for all systems.

In the $\widetilde{T}$-scale was established that behavior of the temperature dependence of the waiting time for first critical nucleus τ_1 is reproduced by single power law

$$\frac{\tau_1(\widetilde{T})}{\tau_1^g} = \left(\frac{\widetilde{T}_g}{\widetilde{T}}\right)^{\gamma}. \tag{11}$$

Here, τ_1^g is waiting time of first critical nucleus at the glass transition temperature T_g, γ is a parameter that characterizes the ability of the system to the structural changes, $\widetilde{T}_g = 0.5$. Also, revealed the presence of correlation in the temperature dependence of $\tau_1(\widetilde{T})$, obtained through a simulation for Dz and bLJ-systems, as well as from experimental data for $Li_2O{\cdot}2SiO_2$, $Na_2O{\cdot}CaO{\cdot}3SiO_2$ and $K_2O{\cdot}TiO_2 \cdot 3GeO_2$ (see figure 2).

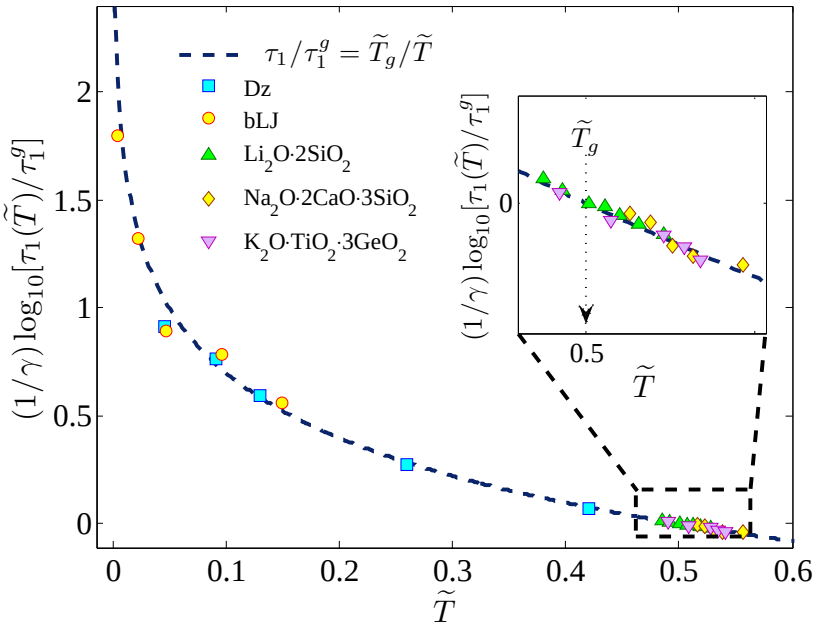

Figure 2: The $(1/\gamma)\log_{10}[\tau_1(\widetilde{T})/\tau_1^g]$ vs. $\widetilde{T}$ curves $\widetilde{T}_g = 0.5$.

It is shown that the power-law dependence of the $\tau_1(\widetilde{T})/\tau_1^g$ summarizes the Abramov-Milchev viscous model,[8] where for the temperature range $0 < T < T_m$ the following relation

$$\log_{10}\left[\frac{\tau_1}{\tau_1^g}\right] = \frac{1}{\ln 10}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\times$$

$$\times\left(\frac{T}{T_g}\right)^{-\gamma n}\left[\left\{2K_1\left(1-\frac{T}{T_g}\right)+\frac{T}{T_g}\right\}^{-\gamma}-\left(\frac{T}{T_g}\right)^{\gamma}\right]^n. \qquad (12)$$

is justly (here, $K_1 = (0.5 - [T_g/T_m]^2)/(1 - [T_g/T_m])$). It is found that the parameter γ correlated with the so-called fragility index

$$m \sim 2\gamma(1 - K_1), \qquad (13)$$

proposed by C.A. Angell for the classification of glasses.[9]

In the fourth chapter presents the results of molecular dynamics simulation the crystallization of the Dz-system at shear deformation. It is shown that the homogeneous shear (Couette-flow) contributes to the appearance of crystalline clusters fcc and hcp lattices. This is confirmed by the time evolution of global orientational order parameter Q_6. In the figure 3 the time dependence of parameter Q_6 is presented for the temperature $T = 0.1\,\epsilon/k_B$ and pressure $P = 14\,\epsilon/\sigma^3$ at shear rate $\dot{\gamma} = 0.001\,\tau^{-1}$ along the axis OX (physical quantities are measured in Lennard-Jones units). It is found that the choice of the optimal value of shear rate and temperature of the system is a key condition for stable crystalline cluster formation and growth.

The numerical evaluation the value of the critical nucleus is performed by method of inverted averaging, where critical size increases from $n_c \simeq 96 \pm 10$ to $n_c \simeq 125 \pm 10$ particles at increase of shear rate and temperature of the system. The calculated dependence of the nucleation rate J_{st} from the shear rate $\dot{\gamma}$ is characterized by a maximum at $\dot{\gamma} \in [0.002;\, 0.005]\,\tau^{-1}$. This indicate that small and moderate shear

[8] I. Avramov, A. Milchev // J. Non-Cryst. Solids. - 1988. - Vol. 104, P. 253.
[9] C.A. Angell // Nature. - 1998. - Vol. 393, P. 521.

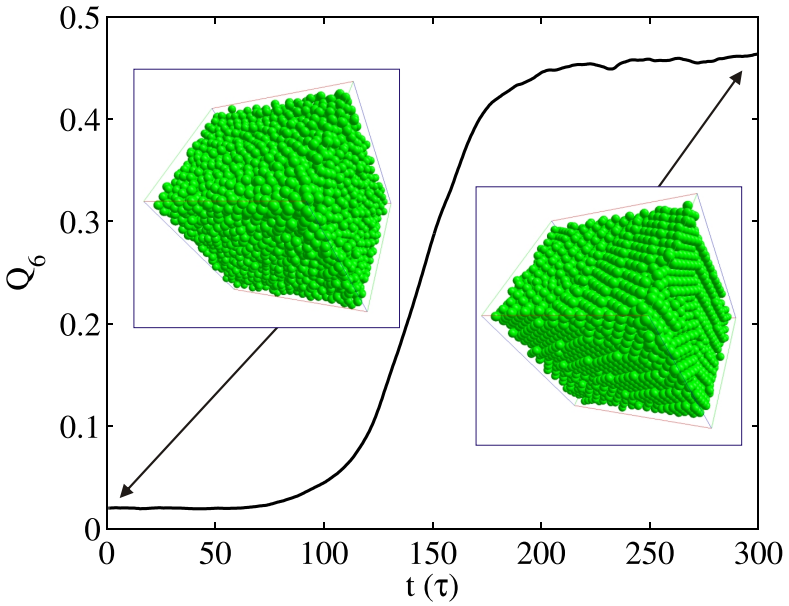

Figure 3: The time dependence of the orientational order parameter Q_6 for Dz-system at shear rate $\dot{\gamma} = 0.001\,\tau^{-1}$ and temperature $T = 0.1\,\epsilon/k_B$. The completely disordered system crystallizes at long time scales.

rates ($\dot{\gamma} < 0.002\,\tau^{-1}$) are increase the nucleation rate. Overly large shear rates ($\dot{\gamma} > 0.005\,\tau^{-1}$) are lead to decrease of the nucleation rate.

It was found that at homogeneous shear of amorphous Dz-system the crystal nuclei become ellipsoidal, where the long axis is oriented in the XY-plane along the shear direction. This is supported by the pair correlation function $g(x, y)$, which calculated for the critical nucleus. The anisotropic growth of the nuclei is caused to discrepancies in the values of the diagonal pressure tensor components P_{xx}, P_{yy} and P_{zz}, which increases with the shear rate (see. table 1). This discrepancy is due to virial contribution in Irving-Kirkwood equation. [10]

[10] D. Reguera, J.M. Rubi J. Chem. Phys. - 2003. - Vol. 119, P. 9888.

Table 1: The values of the diagonal pressure tensor components P_{xx}, P_{xx}, and P_{yy} (in units of ϵ/σ^3) are calculated for various shear rates at temperature $T = 0.15\,\epsilon/k_B$. The values $P_{xx}^{(V)}$, $P_{yy}^{(V)}$, and $P_{zz}^{(V)}$ are determined virial contributions in Irving-Kirkwood equation.

$\dot{\gamma}$, τ^{-1}	P_{xx}	P_{yy}	P_{zz}	$P_{xx}^{(V)}$	$P_{yy}^{(V)}$	$P_{zz}^{(V)}$
0.0001	13.87	14.16	13.98	13.72	14.08	13.83
0.0005	13.87	14.15	13.97	13.72	14.08	13.83
0.001	13.86	14.15	13.97	13.72	14.09	13.83
0.002	13.84	14.21	13.94	13.69	14.10	13.79
0.005	13.76	14.31	13.94	13.61	14.15	13.79
0.008	13.71	14.36	13.92	13.56	14.22	13.77
0.01	13.68	14.41	13.90	13.53	14.26	13.76

In the fifth chapter presents the results of research kinetic and thermodynamic characteristics of the condensation process, which were obtained through molecular dynamics simulation. Here, the possibility of using coarse-grained monatomic (mW) water model for the study of nucleation processes in supersaturated vapor was demonstrated. It is shown that mW-model allows to describe initial stages of condensation in the temperature range from 0°C and 100°C at a pressure of $P = 1$ atm.

The values of the key nucleation parameters as critical size, waiting time, the induction time, were estimated for case of condensation of supercooled vapor. It is shown that the process of condensation accompanied by the formation of droplets of various sizes, consisting of several tens of molecules (see. figure 4). The size of critical droplet decreases from $n_c \simeq 75$ to $n_c \simeq 41$ molecules with increasing temperature in region $0°\text{C} \leq T \leq 100°\text{C}$. At the same time the critical droplets are characterized by a spherical shape, which is confirmed nonsphericity parameter equal to $S_o \simeq 0.008$.

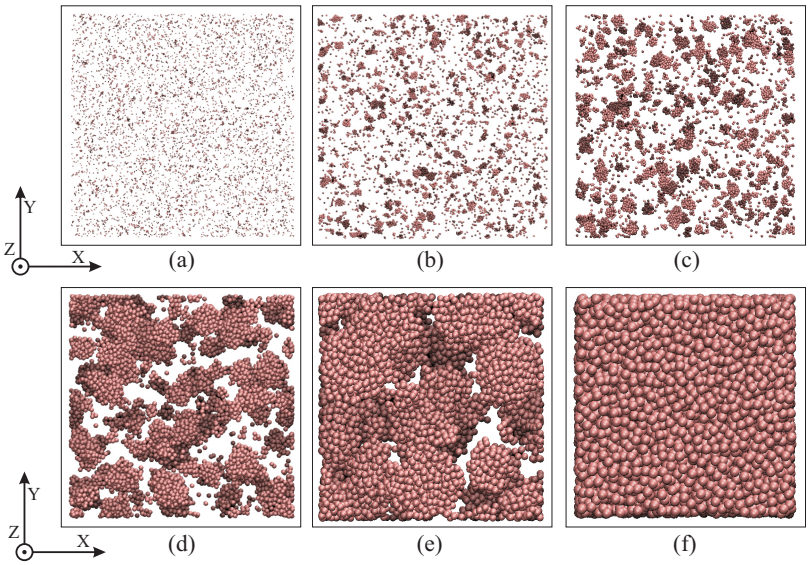

Figure 4: The configurations of system at different time: (a) – $t = 0.3\,\text{ns}$, (b) – $t = 1.0\,\text{ns}$, (c) – $t = 1.1\,\text{ns}$, (d) – $t = 1.2\,\text{ns}$, (e) – $t = 1.25\,\text{ns}$ (f) – $t = 1.3\,\text{ns}$. These results were obtained in temperature $T = 273\,\text{K}$ and pressure $P = 1\,\text{atm}$.

The temperature dependence of the surface tension σ_s of critical droplets is calculated on the based of thermodynamic integration method. The value of $\sigma_s(T)$ are good agreement with the experimental data on compared to the atomistic SPC/E and TIP4P models (see. figure 5). Also, there is shown that the growth of water droplets at condensation is described by a power law, which is unified in considered temperature range. Analysis of growth curves found that growth supercritical droplets is accelerated. This results are completely reproduced by the kinetic theory of Kolmogorov-Johnson-Mehl-Avrami. [11]

Conclusion:

1. The original method of inverted averaging is proposed. This method

[11] A.V. Mokshin, J.-L. Barrat Phys. Rev. E. - 2010. - Vol. 82, P. 021505.

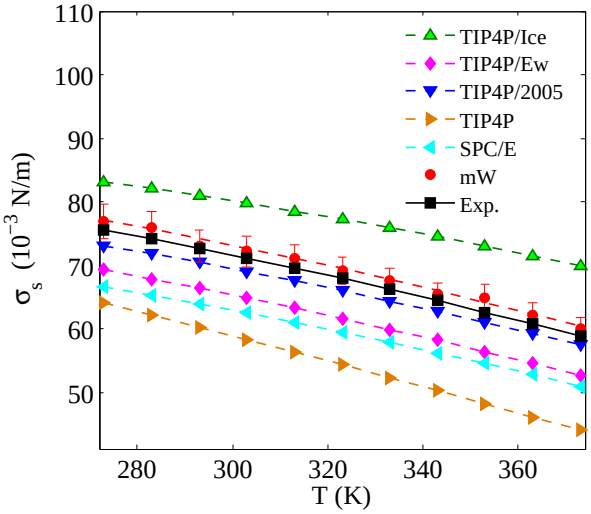

Figure 5: The temperature dependence of surface tension σ_s. With circles the data for mW-model are marked. With square the experimental data are marked. With other markers simulation data for various modifications of atomistic water models SPC/E and TIP4P are designated.

allows to calculate the characteristics of the nucleation and growth processes of a new phase in disordered systems. Also, the approach, which is based on the method of thermodynamic integration is presented. This approach allows to estimate the surface tension of critical nuclei. It is shown that these methods allow to perform the statistical interpretation of the experimental data and results of molecular dynamics simulations.

2. It is shown that the three-particle correlations in multiparticle systems may be considered by method of three-body structural analysis. It is shown that this method allows you to calculate the structural characteristics of the liquid, the amorphous aluminum, and a model of quasicrystal.

3. The original temperature scale was proposed. This temperature

scale allows to compare the nucleation characteristics, which is obtained from experimental data and results of molecular dynamics simulation.

4. It was found that at deep supercooling, as in the case equilibrium and nonequilibrium phase transitions, the crystallization of a one-component and a two-component model glasses occurs through nucleation.

5. The condensation of the supersaturated vapor are investigated by using of coarse-grained water model. It is found that in the case of homogeneous nucleation the growth of water droplets are accelerates growth. The droplets growth laws are uniform in the temperature range from 0°C to 100°C.

Author's publications on the subject of the PhD thesis:

1. Mokshin, A.V. Steady-State Homogeneous Nucleation and Growth of Water Droplets: Extended Numerical Treatment / A.V. Mokshin, B.N. Galimzyanov // J. Phys. Chem. B. - 2012. - Vol.**116,** - P. 11959-11967.

2. Mokshin, A.V. Growth Kinetics of the Homogeneously Nucleated Water Droplets: Simulation Results / A.V. Mokshin, B.N. Galimzyanov // J. Phys.: Conf. Series. - 2012. - Vol.**394,** - P. 012023(1)-012023(4).

3. , .. Ordering in Model Metallic Glass upon External Homogeneous Shear / A.V. Mokshin, B.N. Galimzyanov // Bulletin of the RAS. Physics. - 2013. - Vol.**77,** - P. 281-283.

4. Mokshin, A.V. Extension of Classical Nucleation Theory for Uniformly Sheared Systems / A.V. Mokshin, B.N. Galimzyanov, J.-L. Barrat // Phys. Rev. E. - 2013. - Vol.**87,** - P. 062307(1)-062307(5).

5. Mokshin, A.V. A Method for Analyzing the Non-Stationary Nucleation and Overall Transition Kinetics. A Case of Water / A.V. Mokshin, B.N. Galimzyanov // J. Chem. Phys. - 2014. - Vol.**140,** - P. 024104(1)-024104(6).

6. Mokshin, A.V. Scaling law for crystal nucleation time in glasses / A.V. Mokshin and B.N. Galimzyanov // J. Chem. Phys. - 2015. - Vol.**142,** - P. 104502(1)-104502(10).

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